Transition Energies of Ytterbium ($Z = 70$)

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Transition energies of neutral ytterbium (Yb I, $Z = 70$, belonging to the lanthanide series), including ionization potential, excitation energies, and electron affinity are calculated by the multiconfiguration Hartree–Fock (MCHF) method within the framework of the Breit–Pauli Hamiltonian and the relativistic Hartree–Fock (HFR) method. Ionization potential and excitation energies of Yb II and Yb III are also reported. The obtained results have been compared with other works.

Key words: MCHF Method; HFR Method; Energy Levels; Relativistic Corrections.

1. Introduction

The basic spectroscopic characteristics of an atomic system are the location of the levels (the energies) and the lifetimes (decay probabilities). Unfortunately, present knowledge of these characteristics, in particular for heavy-atom systems, is rather insufficient. This is the case for the rare earths in general [1]. Ionization potentials, excitation energies, and electron affinities are experimentally known for many lanthanides [2]. Ionization potentials are important for identifying physical properties of atoms. The experimental study of negative ions has been a field of intense interest in atomic physics. One aspect of the research on negative ions, determining the electron affinity of an atom, stresses the description of electron correlation in calculations [3].

Relativistic and correlation effects play an important role in wave functions and total binding energies in particular heavy elements. Therefore, an incorporation of the relativistic and correlation effects appears necessary in order to obtain reliable theoretical results for the energies. Relativistic effects, in particular the spin-orbit energy, are a convenient measure to use the relativistic theory for chemical phenomena. Pyykkö and Desclaux [4] determined the importance of relativistic and correlation effects and outlined the mathematical formulation of relativistic quantum theory including the Dirac equation. The relativistic form of the self-consistent field equation was first derived by Swirles [5, 6]. Grant [7] developed a reformulation of the relativistic self-consistent field equations, so that the application to particular problems is simplified. Correlations effects in atoms can often be conveniently split into intravalence, valence-core, and intracore contributions. In ab initio calculations, these contributions can be evaluated by multiconfiguration techniques [8].

Ytterbium is an even-Z rare-earth element ($Z = 70$) with seven natural isotopes, ^{168}Yb (0.13%), ^{170}Yb (3.04%), ^{171}Yb (14.28%), ^{172}Yb (21.83%), ^{173}Yb (16.13%), ^{174}Yb (31.83%), and ^{176}Yb (12.76%). Especially the ytterbium ion has attracted much attention from physicists for several reasons. It has special interest for atomic clocks and trapped-ion frequency standards because the structure of the low-lying levels can be used for optical, infrared or microwave frequency standards [9]. Early theoretical knowledge of lanthanide atoms was presented by Cowan [10]. Worden et al. [11] studied first the ionization potential of lanthanides by laser spectroscopy. Wyart and Camus [12] made analysis of the emission spectrum of neutral ytterbium. Optical-microwave double-resonance spectroscopy of highly excited Rydberg states of ytterbium was studied by Maeda et al. [13]. Yi and co-workers [14, 15] investigated autoionizing states of the ytterbium atom. Baig et al. [16] reported inner shell and double excitation spectra of ytterbium involving the 4f and 6s subshells. Rydberg and autoionizing states of neutral ytterbium were studied by Xu et al. [17]. Wu and co-workers [18, 19] measured some new energy levels belonging to the $4f^{14}6snp\ ^3P_{0,2}$ series of Yb and investigated sixteen autoionizing levels of Yb. Aymar and co-workers [20, 21] investigated high-lying odd-parity levels of Yb I and presented theoretical analysis of highly excited levels of this atom. The interchannel interaction between the single excitation from $4f^{14}$ and the double excitation from $6s^2$ in Yb I was reported by Baig and Connerade [22]. Camus et al. [23] investigated two-photon absorption spectroscopy in ytterbium. Spector [24] identified configurations $4f^{N-1}6s^2 6p$ in Yb. Migdalek and Baylis [8] determined ionization energies and transitions energies for Yb I. Relativistic ionization energies and fine structure intervals of $4f^{14}nl$ states in Yb II were computed including correlation corrections by Koc and Migdalek [25]. The lifetime measurements and calculations of Yb II and Yb III have been investigated by different groups [26 – 30]. A theoretical study of lanthanide atoms was performed by Tatewaki et al. [31]. Sekiya et al. [32] calculated 6s and 4f ionized states of lanthanides by the configuration-interaction method. Transition energies of ytterbium using the relativistic coupled-cluster method were calculated by Eliav et al. [33]. Kotochigova and Tupizin [34] carried out calculations of electronic level structure of rare-earths by the Hartree–Fock–Dirac method. Experimental and theoretical energy levels, transition probabilities, and radiative lifetimes in Yb III were performed by Biémont et al. [35]. Optimized effective potential energies and ionization potentials for the atoms Li to Ra were presented by Gálvez et al. [36]. Nadeau et al. [37] reported the production of stable lanthanide negative ions, also including ytterbium, using accelerator mass spectrometry techniques. Estimations of the electron affinities of lanthanides were made by Bratsch [38]. Electron affinities were tabulated by Hotop and Lineberger [39, 40]. Atomic spectra of rare-earth elements were studied by Meggers [41]. The existence of a stable Yb^- ion with the $4f^{14}6s^2 6p$ configuration was first predicted by Vidolova-Angelova et al. [42]. Gribakina et al. [43] calculated the wave function and binding energy for the outer 6p electron in the negative ion of Yb^- $4f^{14}6s^2 6p$. Electron affinities were evaluated for Yb^- by Avgoustoglou and Beck [44]. Dzuba and Gribakin [45, 46] calculated binding energies and fine-structure intervals for Yb negative ions using the relativistic correlation-potential method and presented strong evidence against the stability of the negative ion of ytterbium. Andersen et al. [47] reinvestigated the previously reported observation of stable negative Yb ions. Predictions of stable Yb^- in the ${}^2P^o{}_{1/2}$ state were presented by Vosko et al. [48]. Litherland et al. [49] observed negative ions of Yb by accelerator mass spectrometry. A list of energy levels for excited levels was compiled and presented by Sansonetti and Martin [50] and can be found on the NIST web site [51].

In this work, we have presented the results including ionization potential and excitation energies of Yb I, Yb II, and Yb III. We have also calculated the electron affinity of atomic ytterbium. The calculations are made by the multiconfiguration Hartree–Fock (MCHF) method within the framework of the Breit–Pauli Hamiltonian [52] and the relativistic Hartree–Fock method (HFR) [10]. Since the basic concepts and features of these methods have been presented at various places elsewhere, here we shall give only a brief account on the theories. The ground-state level of neutral ytterbium is

Table 1. Configuration sets taken in the transition energies (ionization potential (IP) and excitation energies (EE)) calculations for Yb I, Yb II, and Yb III.

	Configurations Yb I	 Yb II	 Yb III
For MCHF + BP calculations			
IP	As in second column for Yb II	As in third column for Yb III	–
EE	$4f^{14}6s^2$, $4f^{14}5d6s$, $4f^{14}6snd$ $(n=6,7)$, $4f^{14}5d^2$, $4f^{14}6p^2$, $4f^{14}6sns$ $(n=7,8)$, $4f^{14}6snp$ $(n=6-9)$, $4f^{14}6snf$ $(n=5,6)$, $4f^{14}5f5g$	$4f^{14}ns$ $(n=6-9)$, $4f^{14}nd$ $4f^{14}ng$, $4f^{14}nf$ $(n=5-9)$, $4f^{14}np$ $(n=6-9)$	$4f^{14}$
For HFR calculations			
IP	As in second column for Yb II	As in third column for Yb III	$4f^{13}$, $4f^{12}6p$, $4f^{12}5d$, $4f^{12}6s$
EE	$4f^{14}6s^2$, $4f^{14}5d6s$, $4f^{14}5d^2$, $4f^{14}6p^2$, $4f^{14}6sns$ $(n=7-12)$, $4f^{14}6snd$ $(n=6-14)$, $4f^{14}6snp$ $(n=6-20)$, $4f^{14}6snf$ $(n=5-15)$	$4f^{14}6s$ $(n=6-11)$, $4f^{13}6s^2$, $4f^{14}nd$ $(n=5-12)$, $4f^{14}ng$ $(n=5,6)$, $4f^{14}np$ $(n=6-12)$, $4f^{13}5d6s$, $4f^{14}nf$ $(n=5-12)$	$4f^{14}$, $4f^{13}np$, $4f^{13}ns$ $(n=6,7)$, $4f^{13}nf$, $4f^{13}nd$ $(n=5-7)$

Table 2. Configuration sets for electron affinity calculations of Yb^-.

For MCHF + BP calculations					
	A	B	C	D	E
Ground-state	$4f^{14}6s^2$, $4f^{14}5d6s$, $4f^{14}5d^2$, $4f^{14}6p^2$, $4f^{14}6s7s$, $4f^{14}6s5g$	$4f^{14}6s^2$, $4f^{14}5d6s$, $4f^{14}6snd$ ($n = 6-9$), $4f^{14}5d^2$, $4f^{14}6p^2$, $4f^{14}6sns$, $4f^{14}5dns$ ($n = 7-9$), $4f^{14}5dnd$ ($n = 6-8$), $4f^{14}5d5g$, $4f^{14}6sng$ ($n = 5-7$), $4f^{14}5g^2$, $4f^{14}6p5f$, $4f^{14}5f7p$, $4f^{14}5f^2$	As in B calculation	As in B calculation	As in B calculation
EA	$4f^{14}6s^2np$, $4f^{14}5d6snp$ $4f^{14}5dns5f$, $4f^{14}5d^2np$ ($n = 6,7$), $4f^{14}5d^25f$, $4f^{14}5d6p7s$, $4f^{14}5d7s7p$, $4f^{14}6s6p7s$, $4f^{14}6s7s7p$, $4f^{14}6p^27p$, $4f^{14}7s^27p$, $4f^{14}np^3$ ($n = 6,7$), $4f^{14}6p7s^2$, $4f^{14}6p7p^2$	$4f^{14}6s^26p$, $4f^{14}5d6s6p$, $4f^{14}5d^26p$	As in A calculation	As in A calculation + $4f^{14}6p5g^2$	$4f^{14}6s^26p$, $4f^{14}5d6s6p$
For HFR calculations					
	A (1.00)	B (2.50)	C (3.00)		
Ground-state	$4f^{14}6s^2$	As in A calculation	As in A calculation		
EA	$4f^{14}6s^26p$	As in A calculation	As in A calculation		

* For HFR calculations, the values in brackets indicate CORRF values. It can be found detail explanations in Section 3.

$6s^2\ {}^1S_0$ of the closed shell formed by the $4f^{14}$ electrons. We have selected various configuration sets according to valence–valence and core–valence (only in HFR calculation) correlations for calculations and presented them in Table 1. Also, configuration sets for the electron affinity calculations of ytterbium are given in Table 2. We reported similar calculations for lanthanum [53, 54] and lutetium [55, 56]. In addition, we presented some radiative properties for ytterbium [57]. The goal of the present work is to contribute to the available atomic data about atomic ytterbium and its anion and cation, and to present them to be used in other experimental and theoretical works in future.

2. Calculation Methods: MCHF and HFR

2.1. MCHF Method

In the multiconfiguration Hartree–Fock method [52], atomic state functions can be obtained as a linear combination of configuration state functions (CSFs) in LS coupling,

$$\Psi(\gamma LS) = \sum_{i=1}^{M} c_i \Phi(\gamma_i LS), \sum_{i=1}^{M} c_i^2 = 1. \qquad (1)$$

The mixing coefficients $\{c_i\}$ and the radial orbitals are optimized simultaneously, based on the expectation values $\langle\Psi|H|\Psi\rangle$.

In the MCHF method, the Breit–Pauli Hamiltonian for relativistic corrections is taken as a perturbation with order α^2. The Breit–Pauli Hamiltonian including relativistic effects can be written as

$$H_{\mathrm{BP}} = H_{\mathrm{NR}} + H_{\mathrm{RS}} + H_{\mathrm{FS}}. \qquad (2)$$

Where H_{NR} is the non-relativistic many-electron Hamiltonian and H_{RS} is the relativistic shift operator including mass correction, one- and two-body Darwin terms, spin-spin contact term, and orbit-orbit term; the fine structure Hamiltonian H_{FS} consists of the spin-orbit, spin-other-orbit, and spin-spin terms. Now, the multiconfiguration wave functions are obtained as linear combinations of CSFs in LSJ coupling. Therefore the radial functions building the CSFs are taken from a previous non-relativistic MCHF run and only the expansion coefficients are optimized. Therefore the matrix eigenvalue problem becomes

$$\boldsymbol{Hc} = E\boldsymbol{c}, \qquad (3)$$

where $\boldsymbol{H}$ is the Hamiltonian matrix with the elements

$$H_{ij} = \langle \gamma_i L_i S_i JM | H_{\mathrm{BP}} | \gamma_j L_j S_j JM \rangle . \tag{4}$$

2.2. HFR Method

In the relativistic Hartree–Fock method [10], for the N electron atom of nuclear charge Z_0, the Hamiltonian is expanded as

$$\boldsymbol{H} = -\sum_i \nabla_i^2 - \sum_i \frac{2Z_0}{r_i} + \sum_{i>j} \frac{2}{r_{ij}} + \sum_i \zeta_i(r_i) \boldsymbol{l}_i \boldsymbol{s}_i \tag{5}$$

in atomic units with the distance r_i of the ith electron from the nucleus and $r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|$. $\zeta_i(R) = \frac{\alpha^2}{2} \left\langle \frac{1}{r} \frac{\partial V}{\partial r} \right\rangle$ is the spin-orbit term with α the fine structure constant and V the mean potential field due to the nucleus and other electrons.

The wave function $|\gamma JM\rangle$ of the Mth sublevel of a level labeled γJ is expressed in terms of the LS basis states $|\alpha LSJM\rangle$ by the formula

$$|\gamma JM\rangle = \sum_{\alpha LS} |\alpha LSJM\rangle \langle \alpha LSJ | \gamma J \rangle . \tag{6}$$

Using determinant wave functions for the atom, the total binding energy is given by

$$E = \sum_i \left(E_{\mathrm{k}}^i + E_{\mathrm{n}}^i + \sum_{j<i} E^{ij} \right), \tag{7}$$

where E_{k}^i is the kinetic energy, E_{n}^i is the electron-nuclear energy, and E^{ij} is the Coulomb interaction energy between electron i and j, averaged over all possible magnetic quantum numbers.

This method calculates one-electron radial wave functions for each of any number of specified electron configurations, using the Hartree–Fock or any of several more approximate methods. It obtains the center-of-gravity energy of each configuration, and those radial Coulomb and spin-orbit integrals are required to calculate the energy levels for the configuration. After the wave functions have been obtained, they are used to calculate the configuration-interaction Coulomb integrals between each pair of interacting configurations. Then, energy matrices are set up for each possible value of J and each matrix is diaganalized to get eigenvalues (energy levels) and eigenvectors (multiconfiguration, intermediate coupling wave functions in various possible angular-momentum coupling representations).

Relativistic corrections to total binding energies become quite large for heavy elements; the main contributions come from the tightly bound inner electrons. In the HFR method, relativistic corrections have been limited to calculations to the mass-velocity and Darwin corrections by using the relativistic correction to total binding energy

$$E_{\mathrm{r}} = \sum_i E_{\mathrm{r}}^i = \sum_i \left(E_{\mathrm{m}}^i + E_{\mathrm{D}}^i \right). \tag{8}$$

3. Results and Discussion

In this work, the transition energies (ionization potentials, excitation energies, and electron affinity) for Yb I, Yb II, and Yb III have been calculated using the MCHF atomic-structure package [58] and Cowan's HFR code [59]. We have considered various configuration sets given in Table 1 according to valence–valence and core–valence (only in HFR calculation) correlations. These configurations include the core [Xe]. Additionally, we have given configuration sets which are taken for the electron affinity calculations of ytterbium in Table 2. The obtained results are reported in Table 3 for Yb I, in Table 4 for Yb II, and in Table 5 for Yb III and are compared with other calculations and experiments in the tables. Ionization potentials and excitation energies are in cm^{-1} whereas electron affinities are in meV. In the tables, the superscript '$^{\mathrm{o}}$' represents the odd-parity states.

Our HFR results are obtained using Cowan's computer code, although the approach is based on the Schrödinger equation, they include the most important relativistic effects like the mass-velocity corrections and Darwin contributions. In these calculations, the eigenvalues of the Hamiltonian were optimized to the observed energy levels via a least squares fitting procedure using the available experimental energy levels. In fact, all the levels taken from the NBS compilation (NIST) were included in the fitting procedure. The scaling factors of the Slater parameters (F^{k} and G^{k}) and of the configuration interaction integrals (R^{k}), not optimized in the least-squares fitting, were chosen equal to 0.75 for Yb I and 0.85 for Yb II, Yb III, and the electron affinity of ytterbium while the spin-orbit parameters were left at their ab initio values. These low values of the scaling factor were suggested by Cowan [10] for neutral heavy elements.

Table 3. Transition energies for Yb I.

Levels		This work		Other works	Leading components (%)	
		HFR	MCHF + BP		HFR	MCHF + BP
			Ionization Potential (cm^{-1})			
$4f^{14}6s^2$	$^1S_0$	49184.10	47229.42 41257.22^*	50441.0^a 41295.25^b 51143^c 48074^d	97.0 + 2.3 $4f^{14}6p^2$ ^1S + 0.4 $4f^{14}5d^2$ ^1S	99.97471 + 0.02528 $4f^{14}6p^2$ ^3P
			Excitation Energies (cm^{-1})			
$4f^{14}6s6p$	$^3P^o_0$	17325.350	17816.72	17288.439^a 17346^c	99.2 + 0.6 $4f^{14}5d6p$ ^3P + 0.1 $4f^{14}6s7p$ ^3P	100.0
	$^3P^o_1$	17945.548	17914.72	17992.007^a 18082^c	96.7 + 2.3 $4f^{14}6s6p$ ^1P + 0.7 $4f^{14}5d6p$ ^3P	99.95463 + 0.04537 $4f^{14}6s6p$ ^1P
	$^3P^o_2$	19718.427	18119.98	19710.388^a 19847^c	98.9 + 0.8 $4f^{14}5d6p$ ^3P + 0.2 $4f^{14}6s7p$ ^3P	100.0
$4f^{14}6s6p$	$^1P^o_1$	25069.266	24593.78	25068.222^a 27283^c	89.1 + 7.2 $4f^{14}5d6p$ ^1P + 2.5 $4f^{14}6s6p$ ^3P	99.95465 + 0.04534 $4f^{14}6s6p$ ^3P
$4f^{14}5d6s$	$^3D_1$	24487.351	24085.73	24489.102^a 24981^c	99.9	100.0
	$^3D_2$	24753.621	24494.30	24751.948^a 25229^c	98.3 + 1.5 $4f^{14}5d6s$ ^1D + 0.1 $4f^{14}6p^2$ ^1D	88.02093 + 11.97421 $4f^{14}5d6s$ ^1D
	$^3D_3$	25271.212	25851.28	25270.902^a 25735^c	99.9	99.99
$4f^{14}5d6s$	$^1D_2$	27668.606	26954.27	27677.665^a 28673^c	89.6 + 7.3 $4f^{14}6p^2$ ^1D + 1.6 $4f^{14}5d6s$ ^3D	87.97825 + 11.96983 $4f^{14}5d6s$ ^3D
$4f^{14}6s7s$	$^3S_1$	32694.747	50254.17	32694.692^a	99.9 + 0.1 $4f^{14}6s8s$ ^3S	100.0
	$^1S_0$	34343.985	51163.44	34350.65^a	97.9 + 0.7 $4f^{14}6s8s$ ^1S + 0.6 $4f^{14}6p^2$ ^1S	99.22644 + 0.077358 $4f^{14}6p^2$ ^3P
$4f^{14}6s7p$	$^3P^o_0$	38068.154	39431.08	38090.71^a	99.1 + 0.5 $4f^{14}5d6p$ ^3P + 0.2 $4f^{14}6s6p$ ^3P	100.0
	$^3P^o_1$	38203.869	39431.08	38174.17^a	98.0 + 1.0 $4f^{14}6s7p$ ^1P + 0.6 $4f^{14}5d6p$ ^3P	100.0
	$^3P^o_2$	38544.364	39431.08	38551.93^a	98.6 + 0.9 $4f^{14}5d6p$ ^3P + 0.3 $4f^{14}6s6p$ ^3P	100.0
$4f^{14}6s7p$	$^1P^o_1$	40563.221	39440.04	40563.97^a	93.7 + 4.2 $4f^{14}5d6p$ ^1P + 1.1 $4f^{14}6s7p$ ^3P	100.0
$4f^{14}6s6d$	$^3D_1$	39807.357	46794.87	39808.72^a	99.9	99.99
	$^3D_2$	39839.630	46794.89	39838.04^a	85.7 + 14.0 $4f^{14}6s6d$ ^1D + 0.1 $4f^{14}5d^2$ ^1D	99.99782 + 0.00208 $4f^{14}6s6d$ ^1D
	$^3D_3$	39966.361	46794.92	39966.09^a	99.9	99.99
$4f^{14}6s6d$	$^1D_2$	40060.175	46800.70	40061.51^a	84.7 + 14.2 $4f^{14}6s6d$ ^3D + 0.5 $4f^{14}5d^2$ ^1D	99.92783 + 0.06983 $4f^{14}6p^2$ ^3P
			Electron Affinity (meV)			
$4f^{14}6s^26p$	$^2P^o_{1/2}$	74.49^A 45.46^B 25.33^C	21.02^A 60.54^B 50.53^C 35.14^D 99.05^E	20^e 45.0^f 36^g 54 ± 27^h 98.5^i	100.0	99.99
	$^2P^o_{3/2}$	7.20^A -80.21^B -113.28^C	-39.23^A -41.61^B 11.79^C -3.55^D 6.15^E	80^e -13.5 ± 27^h 175.5^i	100.0	99.99

[a] [51], [b] [36], [c] [33], [d] [8], [e] [46], [f] [44], [g] [45], [h] [48], [i] [43].

Table 4. Ionization potential and excitation energies of Yb II (in cm^{-1}).

Levels		This work		Other	Leading components (%)	
		HFR	MCHF + BP	works	HFR	MCHF + BP
				Ionization Potential		
$4f^{14}6s$	$^2S_{1/2}$	92513.00	94132.73* 100104.92	98269.00[a] 97934[b] 102764[c1] 95317[c2]	100.0	100.00 99.94* + 0.02 $5p^5 6s6p\ ^2P$ + 0.04 $5p^5 6s6p^4P$
				Excitation Energies		
$4f^{13}(^2F^o)6s^2$	$^2F^o_{7/2}$	21418.700	–	21418.75[a]	100.0	–
	$^2F^o_{5/2}$	31568.099	–	31568.08[a]	99.5 + 0.2 $4f^{13}5d6s(^1F)\ ^2F$ + 0.1 $4f^{13}5d6s(^3F)\ ^4F$	–
$4f^{14}5d$	$^2D_{3/2}$	22960.700	18285.09	22960.80[a] 23770[b] 20333[c2]	100.0	99.99
	$^2D_{5/2}$	24332.700	20044.26	24332.69[a] 25072[b] 21140[c2]	100.0	100.0
$4f^{14}6p$	$^2P^o_{1/2}$	27061.953	20177.41 24390.85*	27061.82[a] 27868[b] 26559[c2]	90.6 + 7.5 $4f^{13}5d6s(^1P)^2P$ + 0.9 $4f^{13}5d6s(^3P)^2P$	100.0 100.0*
	$^2P^o_{3/2}$	30393.883	22103.51 26429.19*	30392.23[a] 31324[b] 29679[c2]	50.0 + 21.6 $4f^{13}5d6s(^3P)\ ^2P$ + 17.2 $4f^{13}5d6s(^3P)^4P$	100.0 100.0*
$4f^{14}7s$	$^2S_{1/2}$	54304.300	85126.80	54304.30[a] 52181[c2]	100.0	100.0
$4f^{14}6d$	$^2D_{3/2}$	62174.100	80957.10 59079.24*	62174.10[a] 59440[c2]	100.0	100.0 99.996*
	$^2D_{5/2}$	62559.100	80962.07 59092.90*	62559.02[a] 59744[c2]	100.0	100.0 99.996*
$4f^{14}7p$	$^2P^o_{1/2}$	63705.387	77001.42	63706.25[a] 60922[c2]	96.5 + 3.0 $4f^{13}5d6s(^1P)\ ^2P$ + 0.3 $4f^{13}5d6s(^3P)\ ^2P$	99.99
	$^2P^o_{3/2}$	65598.211	77002.66	65594.10[a] 62028[c2]	97.9 + 2.0 $4f^{13}5d6s\ (^1P)\ ^2P$	99.99
$4f^{14}5f$	$^2F^o_{5/2}$	70504.300	68441.98	70502.90[a] 67507[c2]	100.0	100.0
	$^2F^o_{7/2}$	70581.400	68443.98	70580.19[a] 67511[c2]	100.0	100.0
$4f^{14}8s$	$^2S_{1/2}$	73039.600	87135.42 70164.50*	73039.6[a] 70488[c2]	100.0	100.0
$4f^{14}8p$	$^2P^o_{1/2}$	76578.499	79117.93	74474[c2]	99.6 + 0.3 $4f^{13}5d6s\ (^1P)\ ^2P$	100.0
	$^2P^o_{3/2}$	77031.801	79118.38	74998[c2]	99.7 + 0.3 $4f^{13}5d6s\ (^1P)\ ^2P$	100.0
$4f^{14}7d$	$^2D_{3/2}$	76517.300	84151.00	76517.21[a]?	100.0	100.0
	$^2D_{5/2}$	76676.300	84153.52	76676.31[a]?	100.0	99.99
$4f^{14}6f$	$^2F^o_{5/2}$	80459.600	73817.05	80458.95[a] 77554[c2]	100.0	100.0
	$^2F^o_{7/2}$	80472.400	73818.38	80471.80[a] 77557[c2]	100.0	100.0
$4f^{14}5g$	$^2G_{7/2}$	80607.500	75554.30	80607.45[a]	100.0	100.0
	$^2G_{9/2}$	80607.500	75554.34	80607.45[a]	100.0	100.0

[a] [51], [b] [36], [c1,c2] [25].

Table 5. Ionization potential and excitation energies of Yb III (in cm^{-1}).

Levels		This work HFR	Other works	Leading components (%) HFR
			Ionization Potential	
$4f^{14}$	$^1S_0$	175045.00	202070.0[a]	$98.5 + 0.5\ 4f^{13}(^2F^o{}_{7/2})5f_{7/2} + 0.3\ 4f^{13}(^2F^o{}_{5/2})5f_{5/2}$
			Excitation Energies	
$4f^{13}(^2F^o{}_{7/2})5d_{3/2}$	$(7/2.3/2)^o{}_2$	33317.696	33385.80[a]	$75.8 + 21.6\ 4f^{13}(^2F^o{}_{7/2})5d_{5/2} + 1.4\ 4f^{13}(^2F^o{}_{5/2})5d_{5/2}$
	$(7/2.3/2)^o{}_5$	37003.304	37020.25[a]	$96.0 + 3.7\ 4f^{13}(^2F^o{}_{7/2})5d_{5/2} + 0.3\ 4f^{13}(^2F^o{}_{5/2})5d_{5/2}$
	$(7/2.3/2)^o{}_3$	39200.109	39141.18[a]	$98.5 + 0.8\ 4f^{13}(^2F^o{}_{5/2})5d_{5/2} + 0.4\ 4f^{13}(^2F^o{}_{7/2})6s_{1/2}$
	$(7/2.3/2)^o{}_4$	39456.473	40160.03[a]	$76.7 + 22.5\ 4f^{13}(^2F^o{}_{7/2})5d_{5/2} + 0.5\ 4f^{13}(^2F^o{}_{5/2})5d_{5/2}$
$4f^{13}(^2F^o{}_{7/2})6s_{1/2}$	$(7/2.1/2)^o{}_4$	34650.593	34656.13[a]	100.0
	$(7/2.1/2)^o{}_3$	34964.007	34990.66[a]	$99.0 + 0.5\ 4f^{13}(^2F^o{}_{7/2})5d_{3/2} + 0.4\ 4f^{13}(^2F^o{}_{7/2})5d_{5/2}$
$4f^{13}(^2F^o{}_{7/2})5d_{5/2}$	$(7/2.5/2)^o{}_6$	38733.010	39085.39[a]	100.0
	$(7/2.5/2)^o{}_1$	39037.476	39720.79[a]	$76.2 + 13.1\ 4f^{13}(^2F^o{}_{5/2})5d_{5/2} + 10.4\ 4f^{13}(^2F^o{}_{5/2})5d_{3/2}$
	$(7/2.5/2)^o{}_2$	41286.128	40288.07[a]	$76.4 + 22.7\ 4f^{13}(^2F^o{}_{7/2})5d_{3/2} + 0.9\ 4f^{13}(^2F^o{}_{5/2})5d_{5/2}$
	$(7/2.5/2)^o{}_4$	41932.308	42425.08[a]	$75.4 + 21.2\ 4f^{13}(^2F^o{}_{7/2})5d_{3/2} + 3.4\ 4f^{13}(^2F^o{}_{5/2})5d_{5/2}$
	$(7/2.5/2)^o{}_3$	42802.880	43019.16[a]	$95.5 + 3.5\ 4f^{13}(^2F^o{}_{5/2})6s_{1/2} + 0.5\ 4f^{13}(^2F^o{}_{5/2})5d_{3/2}$
	$(7/2.5/2)^o{}_5$	43114.705	43622.75[a]	$95.1 + 3.4\ 4f^{13}(^2F^o{}_{7/2})5d_{3/2} + 1.5\ 4f^{13}(^2F^o{}_{5/2})5d_{5/2}$
$4f^{13}(^2F^o{}_{5/2})6s_{1/2}$	$(5/2.1/2)^o{}_2$	44859.109	44853.59[a]	100.0
	$(5/2.1/2)^o{}_3$	45207.292	45207.64[a]	$95.7 + 3.1\ 4f^{13}(^2F^o{}_{7/2})5d_{5/2} + 0.5\ 4f^{13}(^2F^o{}_{5/2})5d_{3/2}$
$4f^{13}(^2F^o{}_{5/2})5d_{5/2}$	$(5/2.5/2)^o{}_0$	45247.509	45276.85[a]?	$99.8 + 0.2\ 4f^{13}(^2F^o{}_{5/2})6d_{5/2}$
	$(5/2.5/2)^o{}_1$	49788.615	50029.42[a]	$50.6 + 25.5\ 4f^{13}(^2F^o{}_{5/2})5d_{5/2} + 23.0\ 4f^{13}(^2F^o{}_{7/2})5d_{5/2}$
	$(5/2.5/2)^o{}_5$	50527.394	50357.46[a]	$98.2 + 1.2\ 4f^{13}(^2F^o{}_{7/2})5d_{5/2} + 0.6\ 4f^{13}(^2F^o{}_{7/2})5d_{3/2}$
	$(5/2.5/2)^o{}_2$	52204.897	51463.38[a]	$96.3 + 1.9\ 4f^{13}(^2F^o{}_{5/2})5d_{3/2} + 1.3\ 4f^{13}(^2F^o{}_{7/2})5d_{5/2}$
	$(5/2.5/2)^o{}_3$	53013.413	53122.79[a]	$91.1 + 7.5\ 4f^{13}(^2F^o{}_{5/2})5d_{3/2} + 0.7\ 4f^{13}(^2F^o{}_{7/2})5d_{5/2}$
	$(5/2.5/2)^o{}_4$	54011.891	53735.86[a]	$94.9 + 4.6\ 4f^{13}(^2F^o{}_{5/2})5d_{3/2} + 0.3\ 4f^{13}(^2F^o{}_{7/2})5d_{3/2}$
$4f^{13}(^2F^o{}_{5/2})5d_{3/2}$	$(5/2.3/2)^o{}_4$	47720.024	47056.92[a]	$91.8 + 4.5\ 4f^{13}(^2F^o{}_{5/2})5d_{5/2} + 1.9\ 4f^{13}(^2F^o{}_{7/2})5d_{5/2}$
	$(5/2.3/2)^o{}_2$	49397.684	48414.67[a]	$96.3 + 2.2\ 4f^{13}(^2F^o{}_{5/2})5d_{5/2} + 1.4\ 4f^{13}(^2F^o{}_{7/2})5d_{5/2}$
	$(5/2.3/2)^o{}_3$	51809.312	51581.78[a]	$91.8 + 7.0\ 4f^{13}(^2F^o{}_{5/2})5d_{5/2} + 0.5\ 4f^{13}(^2F^o{}_{5/2})6s_{1/2}$
	$(5/2.3/2)^o{}_1$	51938.571	53365.19[a]	$63.5 + 36.1\ 4f^{13}(^2F^o{}_{5/2})5d_{5/2} + 0.2\ 4f^{13}(^2F^o{}_{7/2})5d_{5/2}$
$4f^{13}(^2F^o{}_{7/2})6p_{1/2}$	$(7/2.1/2)_3$	72176.654	72140.35[a]	$97.6 + 2.3\ 4f^{13}(^2F^o{}_{7/2})6p_{3/2} + 0.1\ 4f^{13}(^2F^o{}_{5/2})6p_{1/2}$
	$(7/2.1/2)_4$	72482.201	72486.97[a]	$99.4 + 0.6\ 4f^{13}(^2F^o{}_{7/2})6p_{3/2} + 0.1\ 4f^{13}(^2F^o{}_{5/2})6p_{3/2}$
$4f^{13}(^2F^o{}_{7/2})6p_{3/2}$	$(7/2.3/2)_5$	77975.876	78020.45[a]	100.0
	$(7/2.3/2)_2$	78193.816	78183.44[a]	$99.2 + 0.4\ 4f^{13}(^2F^o{}_{5/2})6p_{1/2} + 0.4\ 4f^{13}(^2F^o{}_{5/2})6p_{3/2}$
	$(7/2.3/2)_3$	78777.656	78779.29[a]	$96.9 + 2.3\ 4f^{13}(^2F^o{}_{7/2})6p_{1/2} + 0.8\ 4f^{13}(^2F^o{}_{5/2})6p_{3/2}$
	$(7/2.3/2)_4$	79287.697	79282.90[a]	$99.4 + 0.6\ 4f^{13}(^2F^o{}_{7/2})6p_{1/2}$
$4f^{13}(^2F^o{}_{5/2})6p_{1/2}$	$(5/2.1/2)_3$	82527.268	82546.33[a]	$98.4 + 0.8\ 4f^{13}(^2F^o{}_{5/2})6p_{3/2} + 0.8\ 4f^{13}(^2F^o{}_{7/2})6p_{3/2}$
	$(5/2.1/2)_2$	82894.878	82907.42[a]	$97.9 + 1.6\ 4f^{13}(^2F^o{}_{5/2})6p_{3/2} + 0.5\ 4f^{13}(^2F^o{}_{7/2})6p_{3/2}$
$4f^{13}(^2F^o{}_{5/2})6p_{3/2}$	$(5/2.3/2)_1$	87628.099	87612.61[a]	100.0
	$(5/2.3/2)_4$	88499.501	88497.90[a]	$99.9 + 0.1\ 4f^{13}(^2F^o{}_{7/2})6p_{3/2}$
	$(5/2.3/2)_2$	88983.522	88977.09[a]	$98.0 + 1.7\ 4f^{13}(^2F^o{}_{5/2})6p_{1/2} + 0.3\ 4f^{13}(^2F^o{}_{7/2})6p_{3/2}$
	$(5/2.3/2)_3$	89405.032	89397.41[a]	$99.1 + 0.8\ 4f^{13}(^2F^o{}_{5/2})6p_{1/2}$

[a] [51].

In addition, we have used the MCHF atomic-structure package [58] for the MCHF calculations. In Tables 3 and 4, it is seen that the HFR results are better than the MCHF + BP results when compared with other works. But the MCHF + BP results are not poor except for $4f^{14}6s7s$ and $4f^{14}6s6d$ levels of Yb I. Also, we have performed again the MCHF + BP calculation for Yb II with $4f^{14}5p^6ns$ ($n = 6-9$), $4f^{14}5p^6nd$, $4f^{14}5p^6ng$ ($n = 5-9$), $4f^{14}5p^56snp$ ($n = 5, 6$), $4f^{14}5p^55d7p$, $4f^{14}5p^6np$ ($n = 6-9$), $4f^{14}5p^6nf$ ($n = 5-9$), $4f^{14}5p^55d6s$, and $4f^{14}5p^55d7s$ configuration sets. It is seen that the results from this calculation are only better for the levels of $4f^{14}6p$, $4f^{14}6d$, and $4f^{14}8s$. Ionization potentials of Yb I and Yb II are better with this configuration set, too. These results are indicated with the superscript '*' in the tables. Table 5 is not containing the MCHF + BP results for doubly ionized ytterbium: this code does not allow more than two electrons in a shell with $l \geq 3$. Therefore we have calculated the ionization potential of Yb III with only one configuration, and found it as 169 180.328 cm^{-1}.

In HFR calculations, the quantity CORRF (correction factor) is used as a multiplying factor for a theoretical approximate correlation potential. 1.0 is the theoretically correct value. Physically unreal values greater than unity may be needed for negative-ion calculations [59]. For the electron affinity calculation of ytterbium, we have taken into account different values for CORRF. We have given these values in Table 2.

The formation of stable negative ions of Yb has been the object of many theoretical studies. Different results were obtained in other works. Strong evidence against stability of negative ions of ytterbium was presented and atomic Yb can not form a stable negative ion [46]. We have found various results in both HFR and MCHF + BP calculations for Yb$^-$. The obtained results are in agreement with other works except the 4f^{14}6s^{2}6p ^{2}P$^{o}{}_{3/2}$ level. It should be mentioned that results for Yb$^-$ are very scarce in literature.

In summary, we have calculated the transition energies (ionization and excitation energies and electron affinity) for neutral, the anion, and the cation of atomic ytterbium in the framework of relativistic and correlation effects. As seen in the tables, both MCHF + BP and HFR results for Yb I are in agreement with others. MCHF + BP results are somewhat poor for Yb I and Yb II whereas HFR results agree very well with other works.

We hope that the results reported in this work will be useful for the interpretation of atomic spectra of Yb I, Yb II, and Yb III. Many characteristic features of the spectra of neutral atoms or ions of lanthanides remain preserved for lanthanide ions implemented in crystals. This is one reason for the wide interest in the application of lanthanides as active media in lasers. In addition, knowledge of electronic levels of lanthanides is important in astrophysics, since it allows a precise determination of the abundance of particular elements. Further, the analysis of electronic levels is valuable for a description of the interaction in creating chemical bonds or crystalline lattice. Consequently, we hope that our results using the HFR and MCHF methods will be useful for other works in the future for Yb I, Yb II, and Yb III spectra.

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